

## 2015 Division of Chemistry Annual Newsletter

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## 1. Letter from the Division Director, by David Berkowitz

Greetings Fellow Chemists,

As I write to you, we are sprinting toward the finish line to reach an on time spend-out, so that you can appropriately align personnel and resources to attack fundamental problems at the frontiers of chemistry. I want to lead off this newsletter *en disant* 'merci beaucoup' to Steve Bernasek, Division Director and Linda Sapochak, Acting Deputy Division Director, who led the Chemistry Division (CHE) so adroitly, permitting for a smooth transition at the helm of NSF-CHE. It has been an honor and a privilege to lead the very talented team in the NSF Division of Chemistry and to do so in partnership with Carol Bessel, now officially the permanent Deputy Division Director. Carol has a wealth of knowledge about the academic community, the NSF and the Department of Energy, through her engagement in all of these sectors in her career. Indeed, as I rotate out, I pass the baton to Carol, who will serve as Acting Division Director while the Foundation completes a nation-wide search for Division Director. That search is well underway and an announcement will likely be forthcoming.

It has been an exciting year, with a budget of \$243 million for CHE in FY 2015, a 3.4% increase over FY 2014 (\$236 million). This overall success rate in FY 2014 was 26% and we anticipate a success rate over 20% in FY 2015, as well, and will report the final tallies to you in due course. Over 80% of our budget will go toward funding IIAs (Individual Investigator Awards), the core mission of the Division as we see it. In addition, we remain committed to the Centers of Chemical Innovation (CCI) Program, with the ninth Phase II CCI, the Center for Sustainable Nanoparticles, coming on line this summer. Indeed, ACS President Diane Grob Schmidt sponsored a special ACS Presidential Symposium featuring the NSF CHE CCI Program at the 250<sup>th</sup> National ACS Meeting in Boston on August 16, 2015.

In February 2015, President Obama unveiled his FY 2016 budget request to Congress and this includes a request for an overall 2.2% increase in funding for the Mathematics and Physical Sciences (MPS) Directorate. This would result in an increase to \$251 million for NSF Chemistry (a 3% increase) [http://nsf.gov/about/budget/fy2016/pdf/21\\_fy2016.pdf](http://nsf.gov/about/budget/fy2016/pdf/21_fy2016.pdf). Key elements of the budget request for CHE include: (i) the continuation of Sustainable Chemistry, Engineering, and Materials (**SusChEM**); (ii) extended participation in Cyberinfrastructure Framework for 21st Century Science, Engineering, and Education (**CIF21**); (iii) the continuation of partnerships with the Computer Information Science and Engineering (CISE) and Engineering (ENG) Directorates in **Optics and Photonics**; and (iv) Understanding the Brain (**UtB**), NSF's activity associated with the larger federal BRAIN initiative. UtB will serve as the backdrop for the efforts of a new American Association for the Advancement of Science (AAAS) Fellow, Stephanie Albin, who joins the Division in Fall 2015, fresh from a postdoc at the Howard Hughes Medical Institute (HHMI)-Janelia. Stephanie will be working with the Chemistry of Life Processes (CLP) Program Lead, David Rockcliffe, to examine the scientific space in which chemists can contribute to UtB. Stay tuned!

Finally, perhaps the most notable new program slated for CHE in FY 2016 is **INFEWS** (Innovations at the Nexus at the Food, Energy, Water Systems); CHE will lead the MPS effort in this area, with \$7.2 M requested to support this effort. This program builds on the Food, Energy, and Water (FEW) Dear Colleague Letter (DCL) active in FY 2016. In anticipation of INFEWS, the CHE Division is sponsoring four

FEW workshops, some in partnership with the Chemical, Bioengineering, Environmental and Transport Systems (CBET) Division, under the themes of (i) FEW-Systems Analysis (Organizers: N. Armstrong, A. Barnhart, K. Ogden ); (ii) Closing the Human Phosphorus Cycle (M. Platz, J. Elser) ; (iii) Water (T. Long, F. Bright, P. Edmiston) and (iv) the Nitrogen Cycle (N. Lehnert, G. Coruzzi, L. Seefeldt, E. Hegg). See the full article later in this newsletter for a detailed description of these important workshops. Please look closely at the reports from these workshops as they appear on our website as they will help to define frontier topics for chemists at the food, energy, water nexus. Also, check out the most recent DCL on INFEWS: [http://www.nsf.gov/publications/pub\\_summ.jsp?ods\\_key=nsf15108](http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf15108).

I cannot say enough about the dedication of the CHE technical and administrative staff - the Division is very academic, with hallway discussions about science resembling those at a Gordon Research Conference mixer - animated and active. It is an honor to serve in this setting, with such dedicated and engaged colleagues. Of course, the proposal recommendation process is not easy, with good science always being left on the table. For this reason, the dedicated CHE staff is constantly seeking to leave no stone unturned in the review/award process in availing themselves of appropriate resources to fund as much good science as possible. Our *modus operandi* relies upon broad-based, expert peer review to guide the program director recommendations. These reviews are usually elaborated upon in a dynamic panel discussion as those who have participated in NSF-CHE panel review know well. On behalf of the Division, I want to thank the many members of the CHE community for serving in the reviewer corps. We welcome your feedback on the virtual and in-person panel review processes.

Notably, given the Foundation's working model, the Division is continually looking to renew its rotator core. We seek successful, research-active faculty across all sub-disciplines of chemistry who have an interest in serving the community and experiencing the dynamic setting that is the National Science Foundation, while continuing to lead their research programs through the Individual Research and Development (IR/D) program. You will see, as you read on in this newsletter, that we have an entering group of very talented scientists entering as rotating program directors now. If this speaks to you, please drop us a line and a short curriculum vita.

Lastly, if you plan on being in the neighborhood and would like to talk science, do send us an email and make an appointment to meet with us; contact with program directors is always welcome and is usually meaningful and informative, in both directions. Finally, in a new approach from our end, we may well be in your neighborhood. Namely, as part of a new outreach effort, the CHE Division has visited American Chemical Society (ACS) Regional Meetings in Grand Rapids, Michigan (Great Lakes & Central Regions) and in Pocatello, Idaho (Northwest Region). And, at the 250<sup>th</sup> National ACS Meeting in Boston; NSF Chemistry hosted two events; a poster appearance at the Monday night Sci-Mix (thanks to the Organic Division for facilitating this) as a prelude to the 'Meet the Fed Funders'/Speed Coaching event on Tuesday. In the meantime, best wishes for continued success!

Regards,

David Berkowitz  
Division Director

## 2. Update from the Deputy Division Director, by Carol Bessel

Dear Colleagues,

First and foremost, I would like to add my thanks to both Steve Bernasek, formerly of Princeton University and now of the Yale-National University of Singapore (NUS) College, and David Berkowitz of the University of Nebraska, for their service to the NSF Chemistry Division. Steve served as the CHE Division Director from September 2014 – January 2015 and Dave from February 2015 – July 2015. Both Steve and Dave provided excellent leadership – tirelessly giving of their time in order to help us to develop budget initiatives and drivers, to reach out the community regionally, nationally, and internationally, and to serve the community more effectively and efficiently. The Division greatly appreciates their willingness to "interrupt" their own careers – serving on short notice and facing steep learning curves in six-month rotations. I also thank Linda Sapochak, now the Deputy Division Director in the NSF Division of Materials Research (DMR), for her excellent stewardship of the chemistry portfolio and personnel. Their tremendous dedication to the chemistry community, energy, and enthusiasm for NSF and its mission have been a true inspiration.

At the time of this writing, the Division is in the process of hiring a Division Director. We thank the recent CHE Division Director Search Committee: Melanie Sanford, Joe Francisco, Vicki Grassian, Lisa McElwee-White, Tobin Marks, Tom Mallouk and Steve Zimmerman for their assistance in talking with perspective candidates and answering questions. We have completed the interview process and are looking forward to word of an official appointment. I will be serving as the Acting Division Director till his or her arrival. I also thank Tim Patten, Team Lead for the Chemical Catalysis Program for his willingness to take on the position as Acting Deputy Division Director in the interim.

As Dave mentioned in his letter, in the upcoming month or so, we will be introducing several new staff (Scott Rychnovsky, Carl Carrano and Sarah Stoll), and saying good-bye to some long-time friends and colleagues (Charles Pibel and Fraser Fleming). We have included an Organizational Chart with these changes in this newsletter in order to help you find the appropriate contacts for your proposals.

Please keep an eye out for some new Divisional activities coming in Spring 2016:

- Early Career Investigator Meeting – We will be inviting early career faculty and postdocs interested in academic careers to Washington, D.C. for a special multi-day meeting. Topics will include: proposal writing (CAREER and other), understanding broader impacts, an introduction to NSF programs and CHE personnel, writing reviews for impact, communicating scientific and educational/outreach highlights, mock panels, etc.
- Graduate Education Workshops – In response to our Dear Colleague Letter: Graduate Education in Chemistry (NSF 15-055) the Division is planning two workshops on graduate education. The first will focus on the incorporation of industrial/governmental internships into the graduate student experience and the second will focus on ways to access the various mechanisms for graduate student support (e.g., research assistantships, fellowships, teaching assistantships, internships, etc.)
- Midscale Instrumentation Workshops – We will also be conducting workshops focused on assessing the need for midscale instrumentation in the chemical community. Midscale

instrumentation facilities are significantly larger than those available in from the Major Research Instrumentation (MRI) Program but smaller than the Major Research Equipment and Facilities Construction (MREFC).

If you are interested in these activities, we want you! Please contact me at [cbessel@nsf.gov](mailto:cbessel@nsf.gov).

Finally, we welcome your comments and suggestions, ideas and insights. Please do not hesitate to contact us if we can be of service. Come and see us at our outreach events:

- NOBCCHE Conference in Orlando, FL in September and
- SACNAS Meeting in Washington, DC in October.

Sincerely,

Carol A. Bessel  
CHE Deputy Division Director

### 3. Division of Chemistry Staffing, by Debbie Khalid and Gloria Yancey

**The Division would like to say good-bye and thank you to the following Rotators and Program Directors for their dedication and hard work.** The Division of Chemistry wishes them continued success as they return to their respective universities.

Dr. Catalina Achim, Carnegie Melon University - Chemistry of Life Processes (CLP) Program

Dr. Fraser Fleming, formerly of Duquesne University, now of Drexel University - Chemical Catalysis (CAT) and Chemical Synthesis (SYN) Programs

Dr. Max Funk, University of Toledo - Chemistry of Life Processes (CLP) Program

Dr. Charles Pibel – Chemical Structure, Dynamics and Mechanisms-A, and many other programs. After over 12 years of service to CHE and the chemistry community, Charles will be joining the Department of Chemistry at Georgia Gwinnett College this fall.

#### **The Division welcomes the following new staff members:**

The Division of Chemistry (CHE) welcomes Mrs. Gloria Yancey as the new Program Support Manager (PSM). Gloria comes to CHE from NSF's Behavioral and Cognitive Sciences (BCS) Division where she served as the Administrative Manager for the past six years. Prior to that appointment, she held several career ladder positions at NSF within the CISE, EHR and GEO directorates. Gloria has a Bachelor of Arts degree in English from the University of Maryland Eastern Shore, attended a plethora of career development training classes, and received numerous performance awards including the Director's Award for Administrative Excellence in 2014. The Chemistry Division warmly thanks Mrs. Debbie (Jones) Khalid for serving on a detail assignment as the Program Support Manager during the fall of FY 2014. Debbie did a phenomenal job and we are happy she is staying with us as our Operations Specialist!

Mr. Eric Pfeiffer, joins us as a Program Assistant and is a member of the NSF Pathways Student Intern Program. He currently attends George Mason University.

Dr. Linda Peteanu joins us from Carnegie Mellon University and will be working in the Macromolecular, Supramolecular, and Nanochemistry (MSN) and Chemical Structure, Dynamics, and Mechanisms A (CSDM-A) Programs.

Dr. Anne-Marie Schmoltner is on a one-year detail assignment, as a Program Director in the Chemical Structure, Dynamics & Mechanisms A (CSDM A) Program. Dr. Schmoltner joins CHE from the NSF Atmospheric and Geospace Sciences (AGS) Division.

Dr. Robert Kuczkowski is an Emeritus Professor at the University of Michigan and is assisting Dr. Carlos Murillo in the Major Research Instrumentation (MRI) Program.

Dr. Scott Rychnovsky is rotating in from the University of California-Irvine and will be working in the Chemical Catalysis (CAT) and Chemical Synthesis (SYN) Programs.

Dr. Carl Carrano is rotating in from San Diego State University and will be a Program Director in the Chemistry of Life Processes (CLP) Program.

Dr. Sarah Stoll is rotating in from Georgetown University and will be a Program Director in the Macromolecular, Supramolecular, and Nanochemistry (MSN) and Chemical Synthesis (SYN) Programs.

Dr. George Janini is returning as an Expert to serve as a Program Director in the Chemical Catalysis (CAT) Program.

Finally, we would like to warmly welcome back Dr. Kelsey Cook from his details as: Acting Section Head in the Office of International and Integrative Activities, Staff Associate in the MPS Front Office, and Senior Policy Analyst in the Office of Science and Technology Policy (OSTP). Kelsey will be working in the Chemical Measurement and Imaging (CMI) Program.

#### **4. Innovations at the Nexus of Food Energy and Water Systems (INFEWS) Investment Area, by Colby Foss, Lin He, and Irma Johnson**

Humanity is reliant upon the physical resources and natural systems of the Earth for the provision of food, energy, and water. It is becoming imperative that we determine how society can best integrate across the natural and built environments to provide for a growing demand for food, water and energy while maintaining appropriate ecosystem services. NSF's new investment area, Innovations at the Nexus of Food, Energy, and Water Systems (INFEWS) will stimulate research that: 1) advances our understanding of the complex interactions between food and energy production and water systems, 2) lays the foundations for innovative concepts and technologies that can effectively address the

challenges of resource demands and constraints in food, energy and water systems, and 3) builds a workforce that can realize the goals in 1 and 2. NSF's FY 2016 Budget Request includes \$74.9 million for the INFEWS Investment Area and CHE has requested \$7.2 million of this total.

In preparation for INFEWS in FY 2016 and beyond, the Division of Chemistry has made awards in FY 2015 for four workshops, see below. The reports from these workshops provide researchers in the chemical sciences and engineering with guidance on critical areas of research focus. Investigators are strongly urged to review the outcomes of these workshops (once they are available) on the organizer's website and/or on the NSF CHE website.

In addition, CHE and CBET jointly published a Dear Colleague Letter on August 12, 2015 that identifies topics that are appropriate for INFEWS proposals to the various IIA programs: energy-frugal nitrogen fixation, phosphate sensing, and water purification via processes that are greatly reduced in resource intensity. Proposals on these topics are greatly encouraged in the September and October submission windows. See: [http://www.nsf.gov/about/budget/fy2016/pdf/37\\_fy2016.pdf](http://www.nsf.gov/about/budget/fy2016/pdf/37_fy2016.pdf)

#### **INFEWS Workshops:**

*Addressing the Scientific, Technological and Societal Challenges of the Energy, Water, and Food Nexus: Enabling Resiliency in Energy, Water, and Food Systems for Society*  
April 16-17, 2015, Tucson, AZ

CHE sponsored a workshop on *Addressing the Scientific, Technological and Societal Challenges of the Energy, Water, and Food Nexus: Enabling Resiliency in Energy, Water, and Food Systems for Society* on April 16-17, 2015. The workshop was organized by Professors Neal R. Armstrong and Kimberly Ogden of the University of Arizona, and Program Director Ardeth Barnhart of the University of Arizona Institute of the Environment. The goal of the workshop was to identify the top scientific questions that address the pressing global need to secure the availability of energy, water and food for future generations. See: <http://uanews.org/story/biosphere-2-hosts-forum-on-food-energy-and-water>.

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*FEWS NSF Workshop: Closing the Human Phosphorus Cycle*  
June 8-9, 2015, Arlington, VA

Phosphorus is an element essential to all life. Professor Matthew Platz from University of Hawaii at Hilo and Professor James Elser from Arizona State University co-organized a workshop held on June 8-9, 2015 by bringing together a group of academic, industrial, and governmental scientists to discuss the underlying science that must be advanced to facilitate a more efficient use of phosphorus in food production, as well as the economically viable recovery and recycling of phosphorus at various points in the food system.

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*FEWS NSF Workshop: Food-Energy-Water Systems Challenging Chemists and Chemical Engineers in the 21st Century*

*October 14-15, 2015, Arlington, VA*

This FEWS workshop is co-sponsored by the Chemistry Division and the Chemical, Bioengineering, Environmental, and Transport Systems (CBET) Division. Population growth combined with a concomitant need for more food, energy, and clean fresh water necessitates technological innovations that address a myriad of complex global problems that center on fresh water, the discussion focus of this workshop. This workshop is organized by Professors Timothy Long from Virginia Polytechnic Institute and State University, Frank Bright from the University at Buffalo, and Paul Edmiston from the College of Wooster and will be held on October 14-15, 2015. The workshop aims to bring leading scientists and engineers together to identify the integrated challenges in water research at the water-energy-food nexus.

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*FEWS NSF Workshop: Grand Challenges in the Nitrogen Cycle*

*November 9-10, 2015, Arlington, VA*

CHE and CBET Division co-sponsor a FEWS workshop entitled "*Feeding the World in the 21st Century: Grand Challenges in the Nitrogen Cycle*" on November 9-10, 2015. The nitrogen cycle is one of the most significant biogeochemical cycles on Earth, as nitrogen is an essential nutrient for all forms of life. This workshop will be organized by Professors Nicolai Lehnert from University of Michigan, Gloria Coruzzi from New York University, Eric Hegg from Michigan State University, and Lance Seefeldt from Utah State University. The workshop will bring together scientists from many different areas to define the big scientific challenges in the nitrogen cycle and to develop cross-cutting scientific approaches that could lead to solutions to the identified scientific challenges.

**5. Extreme Science and Engineering Discovery Environment (XSEDE), by: Evelyn Goldfield and Richard Johnson**



The NSF supports a diverse range of high performance computational resources. The Extreme Science and Engineering Discovery Environment (XSEDE), funded from the Advanced Cyberinfrastructure (ACI) Division in the Directorate for Computer and Information Science and Engineering (CISE), provides dynamic distributed infrastructure, support services, and technical expertise that enables researchers to effectively make use of these resources. XSEDE supports a growing collection of advanced computing, high-end visualization, data analysis, and other resources and services.

If your research involves computation of any type (quantum chemistry, molecular dynamics, visualization, large scale data analysis or anything else), we encourage you to investigate how XSEDE can expand your computational horizons. Although XSEDE is funded by the NSF, current NSF funding is not required to apply for an XSEDE allocation. The PI must only be a researcher or educator at a U.S.-



based institution. It is easy to get started: following approval through an on-line application process, the principle investigator (PI) will receive an initial allocation of service units (SUs) and may then add additional group members to the project. *If you do have an NSF award, an initial allocation of resources and/or services is available by submitting the Project Summary for your award along with a 1-2 paragraph description of your needs.*

Network access to XSEDE resources is typically through a secure shell (SSH) protocol. Users need to know a modest number of UNIX commands to work with files and submit jobs for processing, but a high level of computer expertise is not required to access many XSEDE applications. The XSEDE Help Desk provides assistance to users at all levels. *One of the services offered is Extended Collaborative Support, including help with code porting, computational improvements, and data analysis.* Researchers and educators may bring their own software or have access to many common programs for chemistry available across XSEDE networks. To further explore this extraordinary computational resource, see: <https://www.xsede.org/using-xsede>.

## 6. BRAIN Initiative and Understanding the Brain, by David Rockcliffe

In April 2013, the BRAIN Initiative was announced by President Obama. This initiative is intended to stimulate research that would “revolutionize our understanding of the human mind and uncover new ways to treat, prevent and cure brain disorders like Alzheimer’s, schizophrenia, autism, epilepsy, and traumatic brain injury.” NSF’s strategic investments support research and infrastructure designed to transform our view of who we are and how we relate to and interact with each other and our ever-changing environment.

The Chemistry Division has an important role to play in relation to NSF’s brain-related activities and has \$3.80 million to invest in the FY 2016 Request. In order to facilitate the development of significant contributions to the BRAIN Initiative, the Chemistry Division seeks to identify both fundamental chemistry questions and interdisciplinary challenges in which chemists may be able to make important immediate and future contributions to neuroscience and other brain-related research. *Understanding the Brain* activities promise innovative and integrated solutions to challenges in our ability to predict how collective interactions between brain function and our physical and social environment enable complex behavior. CHE welcomes proposals that focus on areas related to designing molecules used in brain imaging and identifying structure-behavior relationships such as those used to interrogate neuronal processes. Please talk to David Rockcliffe ([drockli@nsf.gov](mailto:drockli@nsf.gov)) or your Program Officer if you have research ideas related to understanding the brain. CHE accepts proposals in this investment area during its regular September and October windows.

In this regard, deciphering the operating principles of olfaction requires the development of innovative and integrative approaches that combine novel theoretical frameworks, improved mathematical models, and novel behavioral paradigms across the phylogenetic spectrum, experimental methodologies, and engineering principles. The Biological Sciences (BIO) and Mathematical and Physical Sciences (MPS) Directorates have recently held an Ideas Lab on “Cracking the Olfactory Code” focused on finding innovative solutions to grand challenge problems associated with understanding of

higher-order odor representations and processing during on-going behavior, see [http://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=504773](http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504773). Awards resulting from this Ideas Lab will be made soon.

A recent Dear Colleague Letter on International Collaboration Opportunities related to the NSF Investments in Understanding the Brain has also been published (NSF 14-082): <http://www.nsf.gov/pubs/2014/nsf14082/nsf14082.jsp>.

CHE is enlisting the expertise of an AAAS Fellow, Stephanie Albin, to collect and analyze data and information related to brain research and to develop a community-based activity that would identify the important areas of research at the intersection of chemistry and brain research. Stay tuned!

## **7. Sustainable Chemistry, Engineering, and Materials (SusChEM) Investment Area, by Tingyu Li**

A new FY 2016 Dear Colleague Letter Sustainable Chemistry, Engineering, and Materials (SusChEM) Funding Opportunity was issued on June 4, 2015 (NSF 15-085, [http://www.nsf.gov/publications/pub\\_summ.jsp?ods\\_key=nsf15085](http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf15085)). SusChEM addresses the interrelated challenges of sustainable supply, engineering, production, and use of chemicals and materials. Examples of fundamental research topics of interest in SusChEM include: the replacement of rare, expensive, and/or toxic chemicals/materials with earth-abundant, inexpensive, and benign chemicals/materials; recycling of chemicals/materials that cannot be replaced; development of non-petroleum based sources of important raw materials; chemicals/materials for food and/or water sustainability; the elimination of waste products and enhancement in efficiencies of chemical reactions and processes; discovery of new separation science that will facilitate recycling and production of valuable chemicals/materials; and development and characterization of low cost, sustainable and scalable-manufactured materials with improved properties.

CHE accepts SusChEM proposals in its individual investigator programs (core programs) with windows in September and October 2015. Please contact Tingyu Li ([tli@nsf.gov](mailto:tli@nsf.gov)) if you have questions. To see examples of awards made under the SusChEM, visit the NSF Award Abstracts Database (<http://nsf.gov/awardsearch/>), and enter 'SusChEM' in the 'Search Award for:' dialogue field.

## **8. Designing Materials to Revolutionize and Engineer our Future (DMREF) Solicitation, by Timothy Patten**

The Designing Materials to Revolutionize and Engineer our Future (DMREF) Program is the primary program through which NSF participates in the [Materials Genome Initiative \(MGI\)](#) for global competitiveness. MGI recognizes the importance of materials science to the well-being and advancement of society and aims to "deploy advanced materials at least twice as fast as possible today, at a fraction of the cost." The DMREF Program integrates materials discovery, development, property optimization, and systems design and optimization, with each employing a toolset to be developed within a materials innovation infrastructure. The toolset will synergistically integrate

advanced computational methods and visual analytics with data-enabled scientific discovery and innovative experimental techniques to "revolutionize" our approach to materials science and engineering.

The DMREF Program supports collaborative research activities that build the fundamental knowledge base needed to design and make materials with specific and desired functions or properties from first principles. Achieving this goal will involve modeling, analysis, and computational simulations, validated and verified through sample synthesis and processing, characterization, and device demonstration. It will require new data analytic tools and statistical algorithms; advances in predictive modeling; data infrastructure and reliable, interoperable, and reusable software; and new collaborative capabilities. To cover the breadth of this endeavor, it is expected that DMREF projects will be directed by a team of at least two Senior Personnel with complementary expertise.

CHE participates in DMREF at a level of \$4.00 million in the FY 2016 Request, the solicitation funds awards of three or four years in duration. A new DMREF solicitation is expected out in the Fall of 2015. Please contact Suk-Wah Tam-Chang ([stamchan@nsf.gov](mailto:stamchan@nsf.gov)) or Tim Patten ([tpatten@nsf.gov](mailto:tpatten@nsf.gov)), if you have questions on DMREF submissions.

To see examples of awards made under the DMREF Program, visit the NSF Award Abstracts Database (<http://nsf.gov/awardsearch/>), and enter 'DMREF' in the 'Search Award for:' dialogue field.

## 9. *Chemistry Workshops, by Lin He/Irma Johnson*

Each year the Division hosts a number of workshops on topics of programmatic interest. The following were offered in 2014-2015. Links to the workshop reports will be made to the CHE webpage as they become available.

*Data-Driven Organic Chemistry: Enabling and Innovating the Study of Chemical Reactions*  
September 14-15, 2014, Washington, DC

CHE sponsored a workshop on *Data-Driven Organic Chemistry: Enabling and Innovating the Study of Chemical Reactions* on September 14-15, 2014. The workshop was co-organized by Professor Donna Blackmond from the Scripps Research Institute and Dr. Nicholas Thompson from Pfizer and brought together a group of academic, industrial, and governmental scientists to discuss the more effective and widespread use of in-line analytical techniques to determine reaction pathways and mechanisms, and to explore opportunities for pre-competitive collaborative research between academics and pharmaceutical scientists. The final workshop report can be found at:  
[https://iqconsortium.org/images/Publications/Data\\_Rich\\_Chemistry\\_Report\\_April\\_2015.pdf](https://iqconsortium.org/images/Publications/Data_Rich_Chemistry_Report_April_2015.pdf)

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*Workshop: Mass Spectrometry Big Data To Knowledge*  
May 11-12, 2015, Arlington, VA

The Chemistry Division, Mathematical Sciences Division, and Behavioral and Cognitive Sciences Division co-sponsored a workshop on *Mass Spectrometry Big Data to Knowledge* on May 11-12, 2015. The workshop was organized by Professor John Yates, III, from the Scripps Research Institute. The workshop assessed the current state of proteomic informatics and identified new mathematical and computational frameworks to advance the use of data produced by mass spectrometry. The abstract can be found at: [http://www.nsf.gov/awardsearch/showAward?AWD\\_ID=1349575](http://www.nsf.gov/awardsearch/showAward?AWD_ID=1349575)

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*Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions*  
May 31 - Jun 4, 2015, Arlington, VA

The Macromolecular, Supramolecular, and Nanochemistry (MSN) Program, the Chemical Theory, Models and Computational Methods (CTMC) Program, and the Chemical Structure, Dynamics and Mechanisms A (CSDM-A) Program co-sponsored a workshop on *Accelerating our Understanding of Supramolecular Chemistry in Aqueous Solutions* on May 31 - June 4, 2015. The workshop was organized by Professors Bruce Gibb from Tulane University, Paul Cremer from Pennsylvania State University, Amar Flood from Indiana University, and David L. Mobley from University of California, Irvine and brought together a group of physical scientists who study water and aqueous solutions and supramolecular chemists who investigate non-covalent forces and intermolecular interactions. The workshop catalyzed a deeper development of the fields, generated new ideas and perspectives, fostered a rapid exchange of knowledge between the groups, spurred new collaborations, and ultimately furthered our understanding of the chemistry of aqueous solutions by bridging the knowledge gap between bulk-scale phenomena and the chemical events occurring at the molecular/supramolecular level. The workshop abstract can be found at: [http://www.nsf.gov/awardsearch/showAward?AWD\\_ID=1450865](http://www.nsf.gov/awardsearch/showAward?AWD_ID=1450865)

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*Workshop: Ultrahigh Field NMR and MRI: Science at a Crossroads*  
November 12-13, 2015, Bethesda, MD

The NSF Divisions of Chemistry and Materials Research and the Office of Basic Energy Sciences at DOE are co-sponsoring a workshop on Ultrahigh Field NMR and MRI: Science at a Crossroads, November 12-13, 2015. The workshop is organized by Professor Tatyana Polenova from University of Delaware. The workshop will bring together a group of internationally leading scientists in magnetic resonance to discuss the potential transformative science that will result from High Temperature Superconductor (HTS)-based magnet technologies, as well as the unprecedented opportunities that multiple scientific constituencies could derive from their success. The workshop abstract can be found at: [http://www.nsf.gov/awardsearch/showAward?AWD\\_ID=1547032](http://www.nsf.gov/awardsearch/showAward?AWD_ID=1547032)

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## 10. Computational and Data-Enabled Science and Engineering (CDS&E) Program, by Evelyn Goldfield, Lin He, and Kimberly Noble

The Chemical Measurement and Imaging (CMI) and the Chemical Theory, Models and Computational Methods (CTMC) Programs encourage the submission of CHE Computational and Data-Enabled Science and Engineering (CDS&E) proposals under the Program Description PD 12-8084.

In general, the CDS&E Program welcomes proposals in any area of research supported through the participating divisions that address at least one of the following criteria:

- Promote the creation, development, and application of the next generation of mathematical, computational and statistical theories and tools that are essential for addressing the challenges presented to the scientific and engineering communities by the ever-expanding role of computational modeling and simulation and the explosion and production of digital experimental and observational data.
- Promote and encourage integrated research projects that create, develop and apply novel computational, mathematical and statistical methods, algorithms, software, data curation, analysis, visualization and mining tools to address major, heretofore intractable questions in core science and engineering disciplines, including large-scale simulations and analysis of large and heterogeneous collections of data.
- Encourage adventurous ideas that generate new paradigms and that create and apply novel techniques, generating and utilizing digital data in innovative ways to complement or dramatically enhance traditional computational, experimental, observational, and theoretical tools for scientific discovery and application.
- Encourage ideas at the interface between scientific frameworks, computing capability, measurements and physical systems that enable advances well beyond the expected natural progression of individual activities, including development of science-driven algorithms to address pivotal problems in science and engineering and efficient methods to access, mine, and utilize large data sets.
- innovative and adventurous ideas that generate new paradigms at the algorithmic, software design and data acquisition levels in computational chemistry, simulations, chemical data analysis and cheminformatics, producing new approaches to gaining fundamental chemical knowledge and understanding.

In particular, the Division of Chemistry encourages innovative and adventurous ideas that generate new paradigms at the algorithmic, software design and data acquisition levels in computational chemistry, simulations, chemical data analysis and cheminformatics, producing new approaches to gaining fundamental chemical knowledge and understanding.

A detailed description of the program can be found at [https://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=504813](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504813). Interdisciplinary chemistry proposals with significant CDS&E elements are also encouraged and should be submitted to the most relevant core Chemistry programs with “CDS&E:” labeled in the title. All CDS&E proposals should be submitted within the existing submission window of the selected Chemistry program (September or October). Please contact Evi Goldfield ([egoldfi@nsf.gov](mailto:egoldfi@nsf.gov)) or Lin He ([lhe@nsf.gov](mailto:lhe@nsf.gov)) if you have questions.

## 11. Optics and Photonics, by Carol Bessel

Optics and photonics are key enabling technologies that impact society in a multitude of areas including information and communications, imaging and sensing, healthcare, energy, manufacturing, and national security. With current economic trends of innovation becoming increasingly international, it is a critical time for the NSF to ensure support of fundamental research and disruptive optical technologies that will strongly benefit the nation's scientific and economic health as well as its future workforce. Please look for upcoming announcements in this research area. If you have questions, please contact Linda Peteanu ([lpeteanu@nsf.gov](mailto:lpeteanu@nsf.gov)).

## 12. Outreach Activities

### *American Chemical Society (ACS) Regional Meeting in Grand Rapids, MI, by Michelle Bushey*

Several program officers and staff members from the Chemistry Division and Division of Undergraduate Education (DUE) travelled to Grand Rapids, Michigan for the 6<sup>th</sup> Joint Great Lakes/Central Regional Meeting of the American Chemical Society (ACS) held May 27-30, 2015. NSF staff presented a half-day symposium, conducted a one hour open discussion session and staffed an information booth – answering questions on a variety of topics.

In the half-day symposium, Michelle Jenkins, Program Specialist, opened the session with an overview of the NSF. Program Officer Michelle Bushey then focused on topics most likely to interest future faculty, early career faculty, and new principle investigators. Lin He, Program Officer, addressed funding opportunities that may be less familiar to some in the community, such as:

- Grant Opportunities for Academic Liaisons with Industry (GOALI, NSF 12-513),
- Early-concept Grants for Exploratory Research (EAGER, see NSF Grant Proposal Guide (GPG); [http://www.nsf.gov/pubs/policydocs/pappguide/nsf09\\_1/gpg\\_2.jsp](http://www.nsf.gov/pubs/policydocs/pappguide/nsf09_1/gpg_2.jsp)),
- Grants for Rapid Response Research (RAPID, see GPG),
- Integrated NSF Support Promoting Interdisciplinary Research and Education (INSPIRE, see GPG)
- and Major Research Instrumentation (MRI, NSF-15-504,



[http://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=5260](http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=5260)).

Program Analyst Renee Wilkerson then spoke on opportunities that would be of most interest to undergraduates. Finally, Program Officer, Nicole Bennett of DUE spoke about programs and funding opportunities hosted in the Directorate for Education and Human Resources (EHR).

The open discussion session was well attended and NSF staff fielded questions on a range of topics. The information booth was also popular and many conferees provided their contact information so that they could be considered as reviewers for future proposal submissions.

If you would like NSF staff to attend your regional ACS meeting, please contact Kelsey Cook ([kcook@nsf.gov](mailto:kcook@nsf.gov)) or Carol Bessel ([cbessel@nsf.gov](mailto:cbessel@nsf.gov)).

### ***ACS Regional Meeting in Pocatello, ID, by Kelsey Cook***

On June 21, four itinerant CHE outreachers - administrative staffers Gloria Yancey and Margaret-Anne Wampamba and program officers Carlos Murillo and Kelsey Cook - touched down in Pocatello, Idaho, where they participated in the 69<sup>th</sup> Northwest Regional Meeting of the American Chemical Society (NORM). It was the first visit to Idaho for all four - a metaphor for the newness of Chemistry's efforts to reach out to parts of the community unable to attend our events at the National ACS meetings. Gloria and Margaret-Anne immediately set up the CHE exhibit in time for the Sunday evening welcome event. Meanwhile, Carlos and Kelsey polished the slides for the Monday afternoon Grantsmanship Symposium, featuring NSF overview information (Gloria) and information targeting new faculty (Kelsey), established faculty (Carlos), students/postdocs (Margaret-Anne), and educators (Kelsey and Carlos, using slides provided by the Education and Human Resources Directorate).

NORM is one of the smaller regional meetings (just under 300 attendees, making about 160 technical presentations), and attracted a diverse audience of students and faculty from mainly small colleges and universities, plus disciplinary leaders for symposia on topics that included radiochemistry and chemometrics. Both NSF staff and the meeting attendees had a delightful time interacting together.

### ***ACS National Meeting in Boston, MA Outreach, by C. Renee Wilkerson***

The NSF Division of Chemistry was very actively involved in the 250<sup>th</sup> ACS National Meeting in Boston, MA on August 15-20, 2015.

Several groups invited NSF program staff to join their meetings prior to the start of the National technical program. We thank the Division of Inorganic Chemistry (DIC) and the Division of Physical Chemistry for including us in their "pre-meeting meetings" where we talked about NSF initiatives and rotator recruitment. We also were able to participate in the ACS Postdoc to Faculty Workshop to help near graduates and recent graduates prepare for positions in academic careers.

We thank ACS President Diane Grob Schmidt and Professors Harry Gray and Siddharth Dasgupta of the California Institute of Technology for organizing a special session featuring the National Science Foundation's Centers for Chemical Innovation (CCIs) technical session and poster session on Sunday. This kick-off event highlighted the high impact and innovation of the eight current CCIs.



As a new element in our meeting portfolio, the CHE and CBET Divisions jointly participated in the Sci-Mix Poster session on Monday evening. Posters on NSF CHE programmatic structure and funding opportunities; initiatives and new directions; and broader impacts, broadening participation, education and outreach activities were presented by NSF technical and administrative staff. CHE thanks the ACS Division of Organic Chemistry for including us!

Our big event – the “Federal Funders Symposium & Speed Coaching” session on Tuesday in the Boston Convention & Exhibition Center was a huge success. This event represents an on-going partnership among the National Science Foundation (NSF CHE, Division of Materials Research (DMR), CBET, Division of Molecular and Cellular MCB and Office of International Science and Engineering (OISE)), the Department of Energy (DOE BES), the National Institutes of Health (NIH NIGMS), the Air Force Office of Sponsored Research (AFOSR) and the Environmental Protection Agency (EPA). Each agency/division gave a short presentation on new personnel, budgets, and funding opportunities to a crowd of over 150 ACS attendees.

ACS meeting participants were also able to spend time one-on-one with federal program officers at the annual “speed coaching” session. These 15-minute meetings between attendees and federal funders afforded an opportunity to discuss research ideas, programs, and funding opportunities in depth. More than 250 coaching sessions were held during the afternoon session.

If you haven't participated in the Federal Funders Symposium or the Speed Coaching event, please put us on your calendar as we expect to be back in the Fall of 2016 at the 252<sup>nd</sup> ACS National Meeting in Philadelphia, PA.

***National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) Meeting, by Michelle Jenkins***

The Division of Chemistry will be attending NOBCChE's 42<sup>nd</sup> Annual Meeting, September 21-26, 2015, in Orlando, Florida.

Please stop by and say "hello" as we will be exhibiting at the Career Fair on Wednesday, September 23<sup>rd</sup> from 9:00 am – 2:30 pm. We will have a wide variety of information available on NSF's funding opportunities for students, such as: Chemistry's Research Experiences for Undergraduates (REU)



Program; the Louis Stokes Alliances for Minority Participation Program (LSAMP); and the Graduate Research Fellowship Program (GRFP). In addition to attending the Career Fair, Chemistry's own, Ms. Margaret-Anne Wampamba, is scheduled to talk on “International-Related Activities and Opportunities at NSF,” on Thursday, September 24<sup>th</sup>. This session will be informative for faculty and all students (undergraduate, graduate, and postdoctorals) interested in participating in global activities so please check NOBCChE's website for the time and location.



Last year, Chemistry enjoyed participating in the STEM Weekend Activities, and we are looking forward doing so again.

Please feel free to send an e-mail to: Ms. Michelle Jenkins:

[cjenkins@nsf.gov](mailto:cjenkins@nsf.gov), if you have any questions. CHE is very excited to be a part of another conference as well as working with NOBCChE's terrific staff and committee members! We cannot wait to see everyone soon!

***Society for the Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) Meeting, by: Michelle Jenkins***

The Society for the Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) National Conference motivates, inspires and engages participants to achieve their highest goals in pursuing education and careers in STEM fields. Conference programming is specifically tailored to support undergraduate and graduate students, postdoctoral researchers, and career professionals at each transition stage of their career as they move towards positions of science leadership. The 2015 SACNAS National Conference will be held October 29 - 31 at the Gaylord National Resort & Convention Center in Washington, DC.

The National Science Foundation will have members from the Division of Chemistry attending the upcoming Annual SACNAS National Conference. Further information will be posted to Chemistry's website: <http://www.nsf.gov/chem> in the near future.

**13. CHE Broadening Participation Webpage, by: C.R. Wilkerson**

The Division recently established a Broadening Participation webpage to highlight programs, opportunities, and activities that demonstrate its commitment to broadening participation. Visit the webpage to learn about our outreach activities, funding opportunities, project highlights, special reports and publications, initiatives, and more. We welcome any suggestions and feedback to enhance this important resource for the community! See: [http://www.nsf.gov/mps/che/broadening\\_participation/index.jsp](http://www.nsf.gov/mps/che/broadening_participation/index.jsp)

**14. New NSF Proposal & Award Policies and Procedures Guide (PAPPG), by Marsha Hawkins**

NSF anticipates issuing a revised version of the NSF Proposal and Award Policies and Procedures Guide (PAPPG) in the Fall of 2016. Further details and a copy of the draft NSF PAPPG are available at: <http://www.nsf.gov/bfa/dias/policy>.

**15. CHE Communication ListServ Sign-Up, by C. Renee Wilkerson**

Stay informed with the latest news and topics of interest from the NSF Division of Chemistry: sign up for our mailing list by sending an email message with the subject line, 'Subscribe to CHE', to: [cheminfo@nsf.gov](mailto:cheminfo@nsf.gov). Please share this information with your colleagues!

## 16. International Collaborations: Supplements and Funding Opportunities, by Margaret-Anne Mazzi Wampamba

The Division of Chemistry aims to facilitate collaboration among teams of NSF-supported U.S. scientists and their international partners who have complementary strengths and common interests. While international dimensions may be added to new proposals being submitted to the division, we also invite supplemental requests from our existing awardees who may wish to add a new or strengthen an existing international dimension when such collaboration advances the field of chemistry and enhances the U.S. investigator's own research and/or education objectives. Principal Investigators supported by CHE awards are advised to consult with their Program Officer prior to submitting a supplemental funding request. Supplemental funding proposals for international collaboration should fully address two criteria:

- True intellectual collaboration with foreign research partner; and
- Benefit to the U.S. science/engineering community from expertise, facilities, or resources of the international collaborator.

By clicking on the following link, one can find additional information on NSF programs with international emphasis: <http://www.nsf.gov/mps/che/about.jsp>

- Science Across Virtual Institutes (SAVI): Supports collaboration among teams of NSF-supported U.S. researchers and their international partners wish to form virtual institutes (also has Workforce Development relevance):  
[http://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=504756](http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504756)
- Partnerships for International Research and Education (PIRE): Supports mid-scale awards in which advances in research and education could not occur without international collaboration (also has Workforce Development relevance):  
[http://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=12819](http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=12819)

## 17. NSF Visualization Contest, by Marsha Hawkins

Do you love animating data, creating science apps, or taking macrophotographs? In the Visualization Challenge, aka The Vizzies, sponsored by NSF and *Popular Science*, your handiwork can receive its due reward and you can win cash prizes. The competition aims to recognize some of the most illustrative and impactful visualizations from the worlds of science and engineering. Vizzies participants can



submit their entries in one or more of five categories: Photography, Video, Illustration, Posters & Graphics and Interactive. The Experts' Choice winner in each category will be awarded \$2,500, and the People's Choice winner in each category will be awarded \$500. Expert judges appointed by NSF and *Popular Science* will select a winner (Experts' Choice) in each of the five categories. People's Choice winners will be determined by public votes.

Contest winners will be announced in February 2016, and will be featured in the March issue of *Popular Science*, on popsci.com and <http://www.nsf.gov/news/Vizzies>.

If you have questions, please contact us at [vizzies@nsf.gov](mailto:vizzies@nsf.gov). NSF link: [http://www.nsf.gov/news/special\\_reports/scivis/index.jsp](http://www.nsf.gov/news/special_reports/scivis/index.jsp). Outside link with contest guidelines: <https://app.wizehive.com/apps/nsfvizzies2015>. The deadline for all entries is 11:59 p.m. PST on Sept. 15, 2015.

## 18. Upcoming Proposal Deadlines, by Marsha Hawkins

Chemistry Research Proposals (including unsolicited, Research at Primarily Undergraduate Institutions (RUI) and Grant Opportunities for Academic Liaison with Industry (GOALI)) are due in either the September or October submission windows at 5:00 p.m., submitter's local time, unless otherwise noted.

**Principal Investigators (PIs) may submit proposals to the following programs between Sept. 1 – Sept. 30:**

- Chemical Catalysis - CAT
- Chemical Structure, Dynamics and Mechanisms A - CSDM A
- Chemical Structure, Dynamics and Mechanisms B - CSDM B
- Chemical Theory, Models and Computational Methods - CTMC
- Chemical Synthesis - SYN

**Proposals may be submitted to the following programs between Oct.1 - Oct. 31 to:**

- Chemical Measurement and Imaging - CMI
- Chemistry of Life Processes - CLP
- Environmental Chemical Sciences - ECS
- Macromolecular, Supramolecular and Nanochemistry - MSN

**Major Research Instrumentation Program (MRI) [NSF 15-504](#)**

Proposal submission deadline date: **January 13, 2016**

**Designing Materials to Revolutionize and Engineer our Future (DMREF)**

Keep monitoring the Chemistry Division Webpage for information about DMREF in FY 2016.

## 19. Chemistry Organization Chart, by Marsha Hawkins

<b>Acting Division Director</b>	Carol Bessel
<b>Acting Deputy Division Director</b>	Timothy Patten
<b>Program Support Manager</b>	Gloria Yancey
<b>Operations Specialist</b>	Debbie Khalid
<b>Program Analyst</b>	C. Renee Wilkerson Greaves

## Programs

<b>Chemical Catalysis (CAT)</b> George Janini Marjorie Langell John Gilje Scott Rychnovsky Margaret-Anne Wampamba (Admin. Support)	<b>Macromolecular, Supramolecular and Nanochemistry (MSN)</b> Suk-Wah Tam-Chang Marjorie Langell Linda Peteanu Sarah Stoll Kimberly Noble (Admin. Support)
<b>Chemistry of Life Processes (CLP)</b> David Rockcliffe Carl Carrano Marla Stewart (Admin. Support)	<b>Chemical Measurement and Imaging (CMI)</b> Kelsey Cook Lin He Michelle Bushey Marsha Hawkins (Admin. Support)
<b>Chemical Structure, Dynamics and Mechanisms (CSDM-A)</b> Colby Foss Anne-Marie Schmoltnern Linda Peteanu Illinois Johnson (Admin. Support)	<b>Chemical Structure, Dynamics and Mechanisms (CSDM-B)</b> Tingyu Li Richard Johnson Illinois Johnson (Admin. Support)
<b>Chemical Theory, Models &amp; Computational Methods (CTMC)</b> Evi Goldfield Jim Lisy Kimberly Noble (Admin. Support)	<b>Environmental Chemical Sciences (ECS)</b> Jim Lisy Tyrone Mitchell C. Michelle Jenkins (Admin. Support)
<b>Chemical Synthesis (SYN)</b> Richard Johnson John Gilje Scott Rychnovsky Sarah Stoll C. Michelle Jenkins (Admin. Support)	<b>Major Research Instrumentation (MRI)</b> Carlos Murillo Bob Kuczkowski Marsha Hawkins (Admin. Support)
<b>Chemistry Centers (CENTERS)</b> Kathy Covert Lin He Margaret-Anne Wampamba (Admin. Support)	<b>Undergraduate Programs in Chemistry (REU)</b> Michelle Bushey Tyrone Mitchell C. Michelle Jenkins (Admin. Support)